Odd-even mass difference and isospin dependent pairing interaction

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The neutron and proton odd-even mass differences are studied with Hartree-Fock + BCS (HF + BCS) calculations with Skyrme interactions and an isospin dependent contact pairing interaction, which is recently derived from a microscopic nucleon-nucleon interaction. To this end, we perform HF + BCS calculations for even and odd semi-magic tin and lead isotopes together with even and odd Z isotones with $N = 50$ and 82. The filling approximation is applied to the last unoccupied particle in odd nuclei. Comparisons with the experimental data show a clear manifestation of the isospin dependent pairing correlations in both proton and neutron pairing gaps.

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It has been known that pairing correlations play an important role in finite and also infinite nuclear systems [1–3]. Recently, the theory of nuclear masses or binding energies has attracted renewed interest with the advent of self-consistent mean-field theories and also density functional theories (DFT) [4,5]. A global feature of the nuclear binding energies is the odd-even mass staggering (OES) phenomenon. Several theoretical studies have been made to attribute this phenomenon to the BCS superfluidity in the nuclear ground states. It has been pointed out that other effects also contribute to the OES effect [6,7].

Recently, global calculations of nuclear masses became feasible by using modern computational resources. A goal of these global calculations is to improve the reliability of theories and to establish universal energy density functionals for nuclear masses. In this respect, the pairing correlations should be carefully examined by using microscopic methods such as Hartree-Fock + BCS (HF + BCS) or Hartree-Fock-Bogoliubov (HFB) theories. Indeed, first studies in this direction have been carried out and a possible isospin dependence of the effective pairing interaction has been discussed in the literature [8,9].

The nuclear interaction may conserve the isospin at a fundamental level, but core polarization can induce isospin dependence when the core has a neutron excess. Another contribution may come from the Coulomb interaction. Recently, an effective isospin dependent pairing interaction was proposed from the study of nuclear matter pairing gaps calculated by realistic nucleon-nucleon interactions. In Ref. [8], the density dependent pairing interaction was defined by

$$V_{\text{pair}}(1,2) = V_0 g_\tau[\rho, \beta\tau_z]\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{1}$$

where $\rho = \rho_n + \rho_p$ is the nuclear density and β is the asymmetry parameter $\beta = (\rho_n - \rho_p)/\rho$. The isovector dependence is introduced through the density dependent term g_τ. The function g_τ is determined by the pairing gaps in nuclear matter and its functional form is given by

$$g_\tau[\rho, \beta\tau_z] = 1 - f_s(\beta\tau_z)\eta_s\left(\frac{\rho}{\rho_0}\right)^{\alpha_s} - f_n(\beta\tau_z)\eta_n\left(\frac{\rho}{\rho_0}\right)^{\alpha_n}, \tag{2}$$

where $\rho_0 = 0.16$ fm^{-3} is the saturation density of symmetric nuclear matter. We choose $f_s(\beta\tau_z) = 1 - f_n(\beta\tau_z)$ and $f_n(\beta\tau_z) = \beta\tau_z = [\rho_n(\mathbf{r}) - \rho_p(\mathbf{r})]\tau_z/\rho(\mathbf{r})$. The parameters for g_τ are obtained from the fit to the pairing gaps in symmetric and neutron matter obtained by the microscopic nucleon-nucleon interaction. The pairing strength V_0 will be adjusted to give the best fit to odd-even staggering of nuclear masses.

In the the original EV8 code [10], a pure contact interaction was used without the isospin dependence. In our notation, this amounts to replacing the isospin dependent function g_τ in Eq. (1) by the isoscalar function

$$g_s = 1 - \eta_s\left(\frac{\rho}{\rho_0}\right)^{\alpha_s}. \tag{3}$$

The parameters in this case were adjusted to a best global fit of nuclear masses [11]. They correspond to a surface peaked pairing interaction. Table I shows the parameters for g_τ and g_s used in the present work.

In several previous publications [7–9], the OES was not obtained from the differences of calculated binding energies, but rather was inferred from the average HFB gap parameters. It should be mentioned that the average HFB gaps are sometimes substantially different from the calculated odd-even mass differences. In this work, we compare directly the calculated OES effects with the experimental ones. There are several prescriptions to obtain the OES such as three-point, four-point, and five-point formulas. We adopt the three-point formula $\Delta^{(3)}$ centered at odd nucleus, i.e., odd-N nucleus for neutron gap and odd-Z nucleus for proton gap [2]:

$$\Delta^{(3)}(N,Z) \equiv -\frac{\pi_N}{2}[B(N-1,Z) - 2B(N,Z) + B(N+1,Z)], \tag{4}$$

TABLE I. Parameters for the density dependent function g_τ defined in Eq. (1) (first row) and g_s in Eq. (3). The parameters for g_τ are obtained from the fit to the pairing gaps in symmetric and neutron matter obtained by the microscopic nucleon-nucleon interaction. The paring strength V_0 is adjusted to give the best fit to odd-even staggering of nuclear masses. The parameters for g_s correspond to a surface peaked pairing interaction with no isospin dependence. The parameters in this case are adjusted to a best global fit of nuclear masses [11].

Interaction	V_0 (MeV fm^3)	ρ_0 (fm^{-3})	η_s	α_s	η_n	α_n
g_τ	824	0.16	0.677	0.365	0.931	0.378
g_s	1400	0.16	1.000	1.000	–	–

where $B(N, Z)$ is the binding energy of (N, Z) nucleus and $\pi_N = (-)^N$ is the number parity. For even nuclei, the OES is known to be sensitive not only to the pairing gap, but also to mean-field effects, i.e., shell effects and deformations [6,7]. Therefore, the comparison of a theoretical pairing gap with OES should be done with caution. One advantage of $\Delta_o^{(3)}$ [$N =$ odd in Eq. (4)] is the suppression of the contributions from the mean field to the gap. At a shell closure, the OES (4) does not go to zero as expected, but it increases substantially. This large gap is an artifact due to the shell effect, which is totally independent of the pairing gap itself.

We use the code EV8 [10] to carry out the HF + BCS calculations with Skyrme interactions. The pairing interaction (2) adopted is a contact interaction and can be used in a properly truncated configuration space. In the present study, the energy window is taken as 10 MeV around the Fermi level as is Ref. [10]. This is a limitation of the EV8 code, which solves the HF + BCS equations via a discretization of the individual wave functions on a three-dimensional Cartesian mesh, whereas this program allows flexibility in the determination of the nuclear shape. For a global study of OES, it is important to allow the flexibility of triaxial shapes.

First, the HF + BCS calculations are performed for even-even nuclei. The variables in the theory are the orbital wave functions ϕ_i and the BCS amplitudes v_i and $u_i = \sqrt{1 - v_i^2}$. By solving the BCS equations for the amplitudes, one obtains the pairing energy from

$$E_{\text{pair}} = \sum_{i \neq j} V_{ij} u_i v_i u_j v_j + \sum_i V_{ii} v_i^2, \tag{5}$$

where V_{ij} are the matrix elements of the pairing interaction, Eq. (1), namely,

$$V_{ij} = V_0 \int d^3r |\phi_i(\mathbf{r})|^2 |\phi_j(\mathbf{r})|^2 g_\tau[\rho(\mathbf{r}), \beta(\mathbf{r})\tau_z],$$

where $\rho(\mathbf{r}) = \sum_i v_i^2 |\phi_i(\mathbf{r})|^2$.

In the present study, we take sub-closed shell nuclei only so that the HF minimum appears essentially around the spherical configurations. After determining the single-particle energies of even-even nuclei, the odd-A nuclei are calculated with the so-called filling approximation for the odd particle starting from the HF + BCS solutions of neighboring even-even nuclei: ones selects a pair of i and $\tilde{i}$ orbitals to be blocked and changes the BCS parameters v_i^2 and $v_{\tilde{i}}^2$ for these orbitals. The change is to set $v_i^2 = v_{\tilde{i}}^2 = 1/2$ in Eq. (5) for the pairing energy at an orbital near the Fermi energy. Note that this approximation gives equal occupation numbers to both time-reversed partners and does not account for the effects of time-odd fields. More details of the procedure are presented in Ref. [11].

The effect of time-odd HF fields on the mass were studied in Ref. [12]. It was pointed out that the effect of the time-odd fields is an order of 100 keV for the binding energy depending very much on the configuration of last particle and does not show any clear sign of the isospin dependence. Thus the time-odd field might not change the conclusions of the present study in the following, whereas the quantitative argument might need some fine tuning of the pairing parameters.

The HF + BCS calculations are performed by using SLy4 and SkP Skyrme interactions. The iteration procedure used in EV8 achieves an accuracy of about 100 keV, or less, in 500 iterations. For the pairing channels we take the surface-type contact interaction, Eq. (3), and the isospin dependent interaction, Eq. (2). The density dependence of the latter one is essentially the mixed-type interaction between the surface and the volume types. The pairing strength V_0 depends on the energy window adopted for BCS calculations. The odd nucleus is treated in the filling approximation by blocking one of the orbitals. The blocking candidates are chosen within an energy window of 10 MeV around the Fermi energy. This energy window is rather small, but it is the maximum allowed by the program EV8. It is shown that the EV8 model gives almost equivalent results to the HF + Bogoliubov model with a larger energy window, except for unstable nuclei very close to the neutron drip line [11].

The calculated results are shown in Figs. 1–4. The HF + BCS results are compared with the experimental data and also

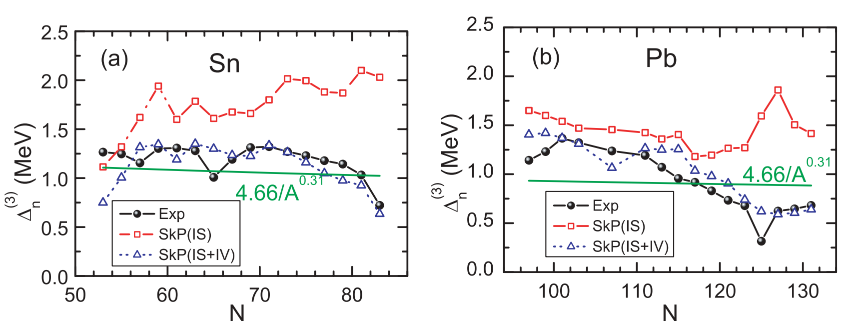

FIG. 1. (Color online) Odd-even mass staggering $\Delta_n^{(3)}$ calculated by Eq. (4) for the semi-magic Sn and Pb isotopes: (a) for Sn isotopes and (b) for Pb isotopes. The SkP interaction is adopted together with the IS pairing (3) or the IS + IV pairing (2) in the HF + BCS model. The filling approximation is applied to the last unoccupied particle in odd nuclei. See the text for details.

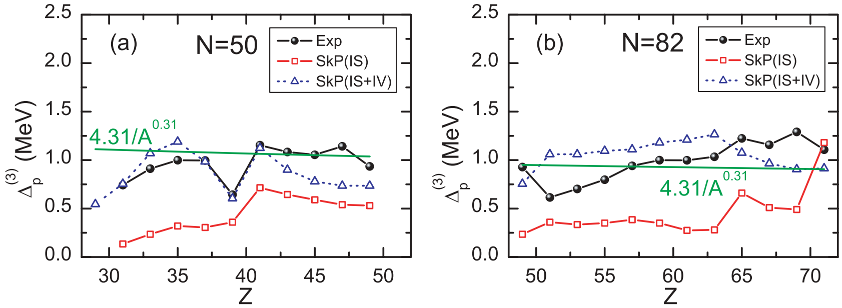

FIG. 2. (Color online) Odd-even mass staggering $\Delta_p^{(3)}$ calculated by Eq. (4): (a) for the $N = 50$ and (b) for $N = 82$ isotones. The SkP interaction is adopted together with the IS pairing (3) or the IS + IV pairing (2) in the HF + BCS model. See the caption to Fig. 1 and the text for details.

the phenomenological parametrization

$$\bar{\Delta} = c/A^{\alpha}, \tag{6}$$

with $c = 4.66$ (4.31) MeV for neutrons (protons) and $\alpha = 0.31$, which gives the rms residual of 0.25 MeV [11].

Figure 1 shows the OES $\Delta_n^{(3)}$ for Sn and Pb isotopes. The calculations are performed with the SkP interaction. The overall agreement with the IS + IV pairing interaction (2) gives quite satisfactory results. Compared with the results with IS pairing (3), the difference is clearly seen in neutron-rich isotopes whereas the difference is rather small in neutron-deficient isotopes. The difference in the two results in larger isospin nuclei is induced by the isospin dependence in Eq. (2), which weakens the pairing strength effectively in neutron-rich nuclei. The experimental OES $\Delta_n^{(3)}$ for Sn isotopes is rather constant around 1.2 MeV until $N = 80$ and deceases below 1 MeV above $N = 82$. This trend is well reproduced by the IS + IV pairing. On the other hand, the calculated results with the IS pairing increase gradually as a function of N and reach up to 2 MeV in heavier Sn isotopes. This feature certainly does not agree with the experimental one. The experimental $\Delta_n^{(3)}$ for Pb isotopes is about 1.4 MeV in neutron-deficient Pb isotopes and goes down to 0.7 MeV in neutron-rich isotopes. This trend is again well accounted for by the IS + IV pairing whereas the IS pairing fails to reproduce this trend in neutron-rich isotopes. The phenomenological gap formula, Eq. (6), gives a good account of overall OES in medium-heavy and heavy nuclei. The average values of $\Delta_n^{(3)}$ for Sn and Pb isotopes are also well reproduced by this formula, but the isospin dependence is relatively weak compared to the experiments and also the IS + IV results, especially in Pb isotopes. In Pb isotopes, the formula gives 0.93 and 0.90 MeV for $N = 99$ and 121 isotopes, respectively, whereas the experimental values are 1.23 and 0.73 MeV for the corresponding isotopes.

In Fig. 2, the calculated proton OES $\Delta_p^{(3)}$ are shown together with the experimental data of $N = 50$ and $N = 82$ isotones. The IS + IV pairing gives again better agreement with the experimental data than with the IS one. Notice that the IS + IV pairing strength becomes larger effectively for smaller Z isotones because of the isospin factor $\tau_z = -1$ for protons in Eq. (2). Quantitatively, the IS pairing gives only about half of the experimental values, and even less than half for the $N = 82$ isotones. On the other hand, the IS + IV pairing provides the proper amount of OES in both $N = 50$ and $N = 82$ isotones because of larger pairing strength for protons in proton-deficient isotones. The kink at $Z = 39$ in Fig. 1 for $N = 50$ isotones is due to the subshell structure at $Z = 40$, which also appeared in the curve of isospin dependent pairing (the white triangles). Equation (6) gives the proton OES to be 1.10 and 1.04 MeV for $Z = 31$ and $Z = 47$ of $N = 50$ isotones, respectively, whereas the experimental values are 0.74 and 1.14 MeV for $Z = 31$ and $Z = 47$ isotones, respectively. We should remind the reader that the Coulomb interaction might play a role for proton OES that is discarded in the present calculations. Some renormalization of the effective pairing strength V_0 might be needed to study the proton OES under the effect of the Coulomb interaction.

In Fig. 3, the IS + IV pairing is tested against another interaction SLy4 for Sn and Pb isotopes. The general features of SLy4 are quite similar to those of SkP except for very neutron-deficient isotopes. This might be because of the small energy window of EV8, but not real physical effects due to the different interactions. Thus the IS + IV pairing works well for OES irrespective of the Skyrme interactions SkP and SLy4.

Recently, different strengths have also been used for neutron and proton pairing interactions with Eqs. (1) and (3) to fit global systematics of masses [11]. As discussed above, Eqs. (1) and (2) do a better job of accounting for the isospin dependence. Nonetheless, it is useful to check how both interactions compare. In Fig. 4, we adopted the different pairing strengths for the surface-type interaction, Eqs. (1) and

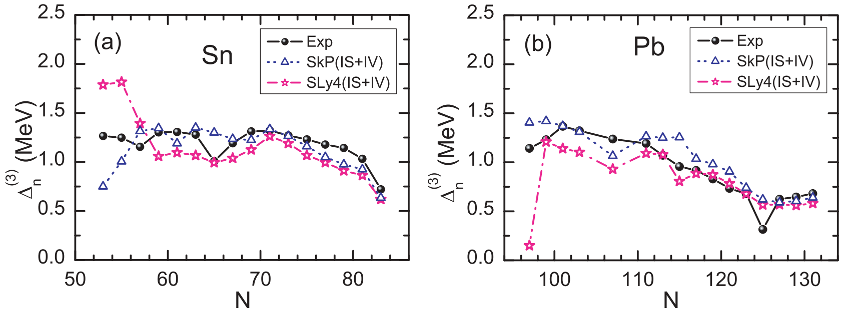

FIG. 3. (Color online) Odd-even mass staggering $\Delta_p^{(3)}$ calculated by Eq. (4): (a) for the $N = 50$ and (b) for $N = 82$ isotones. The SLy4 interaction is adopted together with the IS pairing (3) or the IS + IV pairing (2) in the HF + BCS model. See the caption to Fig. 1 and the text for details.

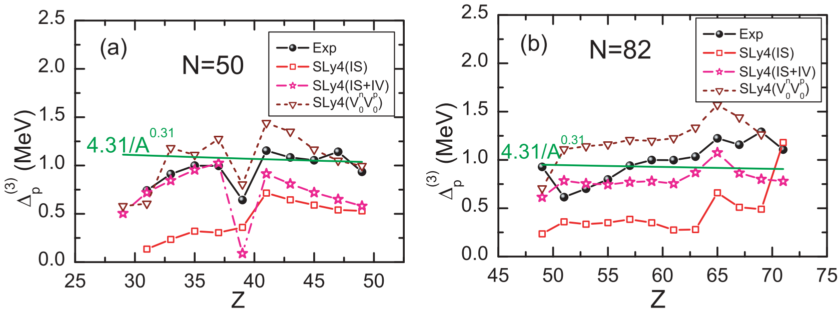

FIG. 4. (Color online) Odd-even mass staggering $\Delta_p^{(3)}$ calculated by Eq. (4): (a) for the $N = 50$ isotones and (b) for the $N = 82$ isotones. The SLy4 interaction is adopted together with the IS pairing (3) or the IS + IV pairing (2) in the HF + BCS model. The different pairing strength $V_0^p = 1462$ MeV fm^3 is adopted in the proton channel for the dotted line with the $V_0^n = 1300$ MeV fm^3 for the neutron channel. See the caption to Fig. 1 and the text for details.

(3), with SLy4 for HF field. We use the same parameters listed in Table I of Ref. [11]: $V_0^p = 1462$ MeV fm^3 for protons and $V_0^n = 1300$ MeV fm^3 for neutrons. The proton $\Delta_p^{(3)}$ values of $N = 50$ and $N = 82$ isotones are shown with three different pairing interactions, IS, IS + IV, and $V_0^p \neq V_0^n$, in Fig. 4. It is seen that $\Delta_p^{(3)}$ is increased substantially for both $N = 50$ and $N = 82$ isotones and gives better agreement with the experimental data than the results of SLy4(IS) in which the proton and neutron pairing strengths were taken to be the same. In Fig. 4(a), both SLy4(IS + IV) and SLy4($V_0^n V_0^p$) show a dip at $Z = 39$ as a sign of subshell structure at $Z = 40$, while the results of SLy4(IS) do not show clear signs of this subshell. For lighter isotones than $Z = 40$, the SLy4(IS + IV) results provide fairly good agreement with the experimental data, but underestimate the data above $Z = 40$. On the other hand, SLy4($V_0^n V_0^p$) gives results close to the experiments for $Z > 45$. We can see that the difference between SLy4($V_0^n V_0^p$) and SLy4(IS + IV) is rather small in small Z isotones and becomes greater in heavier isotones because of the isospin dependence of the pairing strength of the SLy4(IS + IV) model. The general trend of $N = 50$ isotones is the same in $N = 82$ isotones in Fig. 4(b), but to a lesser extent. The results of SLy4($V_0^n V_0^p$) overshoot somewhat the experimental $\Delta_p^{(3)}$, whereas the SLy4(IS + IV) gives slightly smaller values of $\Delta_p^{(3)}$. The small peak at $Z = 65$ reflects the subshell of $Z = 64$. The isotone dependence of experimental $\Delta_p^{(3)}$ of $N = 82$ is better accounted for by SLy4(IS + IV) than SLy4($V_0^n V_0^p$) as can be seen in Fig. 4(b).

In summary, we studied the neutron OES of Sn and Pb isotopes and also the proton OES of $N = 50$ and $N = 82$ isotones by using the HF + BCS model with SkP and SLy4 interactions together with isospin dependence pairing (IS + IV pairing) and IS pairing interactions. The calculations were performed with the EV8 code for even-even nuclei and also for even-odd nuclei using the filling approximation. For the neutron pairing gaps, the IS + IV pairing strength decreased gradually as a function of the asymmetry parameter $[\rho_n(r) - \rho_p(r)]/\rho(r)$. On the other hand, the strength for protons increased for larger values of the asymmetry parameter because of the isospin factor in Eq. (2). The isotope dependence of the neutron OES $\Delta_n^{(3)}$ was well reproduced by the present calculations with the isospin dependent pairing compared with the IS pairing. We also saw good agreement between the experimental proton OES and the calculations with the isospin dependent pairing for $N = 50$ and $N = 82$ isotones.

We tested the IS + IV pairing for the Skyrme interaction SkP and found almost the same quantitative agreement as with SLy4; i.e., the results reproduced well the experimental data of Sn and Pb isotopes. Thus, we confirm the clear manifestation of the isospin dependence of the pairing interaction in the OES in comparison with the experimental data for both protons and neutrons. More comprehensive study of OES in the entire mass region is planned as a future work.

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